

1-Hexadecanol  
36653-82-4 | DTXSID4027991

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 9.67e-08 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.55e-01

Confidence level: 5.73e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Hexadecanol</div> <div>Measured: 9.69e-08</div> <div>Predicted: 9.67e-08</div>	<div>Image not found</div> <div>Heptadecan-1-ol</div> <div>Measured: 3.12e-08</div> <div>Predicted: 4.13e-08</div>	<div>Image not found</div> <div>1-Pentadecanol</div> <div>Measured: 4.48e-07</div> <div>Predicted: 2.58e-07</div>
<div>Image not found</div> <div>1-Octadecanol</div> <div>Measured: 4.07e-09</div> <div>Predicted: 1.32e-08</div>	<div>Image not found</div> <div>1-Tetradecanol</div> <div>Measured: 1.12e-06</div> <div>Predicted: 8.26e-07</div>	